Merck Index 13th Edition Page 1693 S-(+)-Form hydrochloride. [53984-76-2] Crystals from ethanol-diethyl ether, mp 264.5°. $[\alpha]_D$ +42.35° (c = 2.63 in methanol).

THERAP CAT: Antiarrhythmic (class IB).

9569. Tocamphyl. [5634-42-4] 1,2,2-Trimethyl-1,3-cy-clopentanedicarboxylic acid 1-[1-(4-methylphenyl)ethyl] ester, compd with 2,2'-iminobis[ethanol] (1:1); camphoric acid 1- $(p,\alpha$ -dimethylbenzyl) ester, compd with 2,2'-imidodiethanol (1:1); p,α -dimethylbenzyl camphorate diethanolamine salt; p-toluoylmethylcarbinolmono-d-camphoric acid ester diethanolamine salt; p-tolylmethylcarbinol camphorate diethanolamine salt; p-tolylmethylcarbinol camphorate diethanolamine salt; diethanolamine p-tolylmethylcarbinol camphorate; diethanolamine d-methyltoluylcarbinol camphorate; Biliphorine; Hepatoxane; Syncuma. $C_{23}H_{37}NO_6$; mol wt 423.54. C 65.22%, H 8.30%, N 3.31%, O 22.67%. Prepn: CH 211203 (1940 to Chemiewerk Homburg); Chem. Zentr. 1941, I, 2972.

Crystals, sol in water. THERAPCAT: Choleretic.

9570. Tocol. [119-98-2] 3.4-Dihydro-2-methyl-2-(4.-8.12-trimethyltridecyl)-2H-1-benzopyran-6-ol; 2-methyl-2-(4.-8.12-trimethyltridecyl)-6-chromanol; 2-methyl-2-phytyl-6-chromanol; 6-hydroxy-2-methyl-2-phytylchroman; 2-methyl-2-phytyl-6-hydroxychroman. C₁₀H₁₄O₂; mol wt 388.62. C 80.36%. H 11.41%, O 8.23%. Synthesis by the condensation of hydroquinone and phytol in the presence of anhydr formic acid: Pendse, Karrer, Helv. Chim. Acta 40, 1837 (1957). Antioxidant activity of tocol and its methyl derivs: Olcott, van der Veen. Lipids 3, 331 (1968).

Colorless, viscous oil, bp_{0.001} 165-175°, Acetate, $C_{28}H_{16}O_4$, Viscous oil, bp_{0.001} 180-185°, tSE: Antioxidant.

9571. α-Tocopherol. [59-02-9] (2R)-3,4-Dihydro-2,-5.7.8-tetramethyl-2-[(4R,8R)-4.8,12-trimethyltridecyl]-2//-1benzopyran-6-ol; (+)-2,5,7,8-tetramethyl-2-(4',8',12'-trimethyltridecyl)-6-chromanol: R.R.R-\alpha-tocopherol; d-\alpha-tocopherol; 5,7.8-trimethyltocol: Optovit: Tocovital. C20H50O2: mol wt 430.70. C 80.87%, H 11.70%, O 7.43%. Most bioactive of the naturally occurring forms of vitamin E, q.v. Richest sources are green vegetables, grains, and oils, particularly palm, safflower and sunflower oils. Isoln from wheat germ: H. M. Evans et al., J. Biol. Chem. 113, 319 (1936). Structure: E. Fernholz, J. Am. Chem. Soc. 59, 1154 (1937); 60, 700 (1938). Synthesis of dlform: P. Karrer et al., Helv. Chim. Acta 21, 520, 820 (1938): F. Bergel et al., J. Chem. Soc. 1938, 1382. Distillation from vegetable oils and prepn of esters: J. G. Baxter et al., J. Am. Chem, Soc. 918 (1943). Prepn of crystalline natural form: C. D. Robeson, ibid. 1660; of crystalline acetate: idem, ibid. 64. 1487 (1942). Abs config of natural α -tocopherol: H. Mayer et al., Helv. Chim. Acta 46, 963 (1963). Stereoselective synthesis: K.-K. Chan et al., J. Org. Chem. 43, 3435 (1978). Total synthesis of all 8 stereoisomers: N. Cohen et al., Helv. Chim. Acta 64, 1158 (1981). Clinical trial in Alzheimer's disease: M. Sano et al., N. Engl. J. Med. 336, 1216 (1997); to improve immune function in healthy elderly: S. N. Meydani et al., J. Am. Med. Assoc. 277, 1380 (1997). Review of bioavailability from vitamin E supplements: M. G. Traber. BioFactors 10, 115-120 (1999). Review of clinical trials in heart disease: W. A. Pryor, Free Radical Biol. Med. 28, 141-164 (2000).

Transparent needles, mp 2.5-3.5°. $[\alpha]_{546.1}^{25}$ +0.32° (benzene); $[\alpha]_{546.1}^{25}$ +0.32° (ethanol).

Acetate. [58-95-7] Spondyvit. $C_{31}H_{52}O_{3}$; mol wt 472.74. Light yellow oil. Crystallized at -30° as needle-like crystals, mp 26.5-27.5°. $[\alpha]_D^{25} + 0.25^{\circ}$ (c = 10 in chloroform); $[\alpha]_D^{15} + 3.2^{\circ}$ (in ethanol).

Succinate. [4345-03-3] $d-\alpha$ -Tocopheryl acid succinate; Tocovite. Needles from petr ether, mp 76-77°. uv max (ethanol): 286 nm (E_{loo}^{18} 38.5). Practically insol in water.

 $dl \cdot \alpha$ -Tocopherol. [10191-41-0] all-rac- α -Tocopherol. Equimolar mixture of all four racemates. Slightly viscous, pale yellow oil. d_s^{25} 0.950; $bp_{0.1}$ 200-220°; n_s^{25} 1.5045. uv max: 294 nm (E_{loo}^{13} , 71). Practically insol in water. Freely sol in oils, fats, acctone, alcohol, chloroform, ether, other fat solvents. Stable to heat and alkalies in the absence of oxygen. Not affected by acids up to 100°. Slowly oxidized by atm oxygen, rapidly by ferric and silver salts. Gradually darkens on exposure to light.

dl-α-Tocopherol acetate. [52225-20-4] dl-α-Tocopheryl acetate: Detulin; Ephynal; Eusovit; Evion. Comprehensive description: B. C. Rudy. B. Z. Senkowski, Anal. Profiles Drug Subs. 3, 111-126 (1974). Pale yellow, viscous liquid. mp -27.5°. d₄^{21.3} 0.9533. bp_{0.01} 184°: bp_{0.025} 194°: bp_{0.3} 224°. n₅²⁰ 1.4950-1.4972. uv max (cyclohexane): 285.5 nm. Practically insol in water. Freely sol in acetone, chloroform. ether. Less readily sol in alc.

USE: As an antioxidant in vegetable oils and shortening. THERAP CAT: Vitamin E supplement.

THERAP CAT (VET): Vitamin E supplement.

9572. β -Tocopherol. [16698-35-4]: [148-03-8] (dl-form). (2R)-3.4-Dihydro-2.5.8-trimethyl-2-[(4R.8R)-4.8.12-trimethyltridecyl]-2H-1-benzopyran-6-0l: (+)-2.5.8-trimethyl-2-(4.8.12-trimethyltridecyl)-6-chromanol: 5.8-dimethyltocol: cumolocopherol: neotocopherol: p-xylotocopherol. $C_{28}H_{48}O_2$: mol wt 416.68. C 80.71%, H 11.61%, O 7.68%. One of the naturally occurring forms of vitamin E, q-v. Is biologically less active than α -tocopherol. May be separated by fractional crystn: Emerson et al., Science 83, 421 (1936); J. Biol. Chem. 113, 319 (1936); Baxter et al., J. Am. Chem. Soc. 65, 918 (1943).

Pale yellow, viscous oil. $bp_{0,1}$ 200-210°. $[\alpha]_{366,1}^{25}$ +2.9° (c = 7.15 in ethanol). uv max: 297 nm (E_{lom}^{13} 87.6). Insol in water. Freely sol in oils, fats, acetone, alcohol, chloroform, ether, other fat solvents. Very stable to heat and alkalies. Slowly oxidized by atmospheric oxygen, rapidly by ferric and silver salts. Gradually darkens on exposure to light.

9573. γ-Tocopherol. [54-28-4]: [7616-22-0] (dl-form). (2R)-3,4-Dihydro-2.7.8-trimethyl-2-[(4R.8R)-4.8.12-trimethyl-tridecyl]-2H-1-benzopyran-6-ol; (+)-2.7.8-trimethyl-2-(4.8.12-trimethyltridecyl)-6-chromanol; (R.R.R)-γ-tocopherol: 7.8-dimethyltocol: σ-xylotocopherol. C_{2n}H_{4n}O₂: mol wt 416.68. C 80.71%. H 11.61%. O 7.68%. One of the naturally occurring forms of vitamin E, q.v. Most abundant tocopherol in soybean and corn oils. Isoln by fractional crystn: Emerson et al., Science 83, 421 (1936); J. Biol. Chem. 113, 319 (1936); J. G. Baxter et al., J. Am. Chem. Soc. 65, 918 (1943). Prepn of crystalline natural form: C. D. Robeson, J. Am. Chem. Soc. 65, 1660 (1943). Comparison of bioactivity with α-tocopherol, q.v.: J.